#### **50. REMOTE SENSING**

For decades, the Remote Sensing Program has been a cornerstone in the national capability for the detection of facilities and activities related to the proliferation of foreign nuclear programs. The Remote Sensing Program research projects encompass a wide variety of potential capabilities to detect signatures associated with the development of nuclear weapons. The research areas in the Remote Sensing program include sensor development, image processing, and digital signal processing techniques for characterization of observed phenomena.

# 50a. Improvement in Quality of II-VI and III-V Semiconductor Materials for IR Focal Plane Arrays

The ability to grow defect-free materials could conceivably enhance the performance and reliability of constituent photodiodes in II-VI and III-V infrared imaging focal plane arrays, such as HgCdTe and Sb-based SLS. As in any semiconductor device, elimination of defects and anomalies in the underlying material system will enhance device quality and performance, yielding improved focal plane arrays. Applications are sought to enable refinements in focal plane array technology, systematically and routinely through any relevant strategies, including but not limited to, application of advanced analytical imaging methodologies and evaluation of the impact of defects and anomalies on FPA performance and lifetime. Partnership with II-VI / III-V vendors or National Labs may be desirable to access sample test articles.

Contact: Victoria Franques, 202-586-2560, victoria.franques@nnsa.doe.gov

## 50b. Thermal Mitigation for IR Detectors

Applications are sought to develop advanced thermoelectric or other non-vibrational, low-power cooling systems capable of bringing temperatures in a one inch square area producing 5W of heat down from ambient to 77K at high efficiency. The next-generation MWIR and LWIR imaging systems still require cooling of detectors and back focal assemblies to reduce self-emission and improve sensitivity. Current conventional cooling systems (such as Sterling Cycle coolers or refrigerant gases) are bulky and/or introduce additional vibration, heat, and power consumption into the system.

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## 50c. Waveguide-Coupled Optical Modulator for W-Band Up-Conversion

Passive millimeter wave imaging provides many advantages in remote sensing, such as the ability to see through clouds, dust, and smoke, as well as daytime/nighttime operation. One atmospheric window that is exploited in millimeter wave imaging is at 94GHz (W-band). However, a potential drawback with passive millimeter wave imaging is its inherent low resolution compared to optical approaches, such as passive infrared imaging. Therefore, at reasonable standoff distances, sub-pixel detection methods, or exploitation of mixed pixel data, become essential. One approach to extracting additional information is the use of millimeter wave polarimetry. However, this approach requires the polarization signals to be combined

coherently, which can cause the very sensitive components used in CMB (Waveguide-coupled optical Modulator for W-band) research to suffer significant waveguide loss in signal routing. This drawback can be alleviated by optical up-conversion, while still preserving the amplitude and phase relationship of multiple signals. Moreover, optical up-conversion would provide other benefits: (1) it would enable advances in optical components, which result from the telecomm build-out, to be leveraged; and (2) it would permit remote operation of two or more receivers in a phased array, in order to increase imaging resolution. Unfortunately, no commercial full-band W-band (75-110 GHz) modulators exist presently, although research suggests steady improvement in the fabrication of research devices. Therefore, to advance instrument development in passive millimeter wave imaging for remote sensing applications, grant applications are sought for the design and fabrication of a low-insertion-loss W-band modulator having a mm-wave insertion loss of < 2.5dB and an optical insertion loss of < 3dB.

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#### 50d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas relevant to this Topic.

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- 2. Richard Martin, et al., "Design and Performance of a Distributed Aperture Millimeter-Wave Imaging System Using Optical Upconversion", Proc. SPIE, Vol. 7309, 730908-1, (2009). (Full text available at: http://spiedl.aip.org/dbt/dbt.jsp?KEY=PSISDG&Volume=7309&Issue=1)
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## 51. RADIATION DETECTION

The Office of Nuclear Nonproliferation Research and Development (NA-22) is focused on enabling the development of next generation technical capabilities for radiation detection of nuclear proliferation activities. As such, the office is interested in the development of radiation detection techniques and sensors, and advanced detection materials, that address the detection and isotope identification of unshielded and shielded special nuclear materials, and other radioactive materials in all environments. In responding to these challenging requirements, recent research and development has resulted in the emergence of radiation detection materials that have good energy resolution. From these materials, the development of radiation detectors that are rugged, reliable, low power, and capable of high-confidence radioisotope identification

are sought. Currently, the program is focused on the development of improved capabilities for both scintillator- and semiconductor-based radiation detectors. The objective of this topic is to gain insight into a mechanistic understanding of material performance as the base component of radiation detectors. That is, the program is interested in moving beyond the largely empirical approach of discovering and improving detector materials to one based on a clear understanding of basic materials properties.

## 51a. Scintillators for Gamma Spectroscopy

We would like to support research on materials that will lead to practical high-brightness scintillators with energy resolution significantly better than the currently available sodium iodide-based gamma spectrometers. Several new and promising formulations have been discovered and synthesized in small quantities, but there is a need for industrial crystal-growth facilities to find ways to produce practical sizes of high-quality scintillators at a reasonable cost. As an alternative to crystal growth, techniques that produce high quality, large volume scintillators with good spectroscopic performance from the consolidation of powders are highly desirable. Although most previous work has been done with oxide compounds, polycrystalline halide scintillators – formed from the new alkaline earth halides, the elpasolites, and other materials that demonstrate high performance in single-crystal form – would be of particular interest. It is important to incorporate elements with high atomic number in order to enhance the photoelectric effect. Also, a scintillator thick enough to absorb high energy gamma rays must also be very transparent to its own emitted light. A laboratory demonstration is expected in Phase I, while Phase II should lead to the development of a commercial process with a significant advantage over current crystal growth techniques.

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## 51b. Semiconductors for Gamma Spectroscopy

We are interested in promoting the industrial capacity to develop large volume, high quality radiation detector materials based on semiconductors. As an example, in the last three years, pixelated cadmium zinc telluride (CZT) detectors using depth correction have demonstrated resolution at room temperature (0.5% at 662 keV) that rivals high purity germanium (HPGe). Approaches of interest must address growth issues involving such semiconductor materials, so that reliable, high yield, rapid, and large volume growth is readily achievable at a reasonable cost. It should be recognized that good electronic transport properties are essential, such as electron and hole mobilities and lifetimes, which as a rule require extremely low concentrations of deleterious impurities and careful control of deliberate dopants. Phase I should result in the identification of a clear path to improving upon existing growth techniques. Phase II should include a demonstration of a material fabrication process that is free from dislocations, cracking, chemical heterogeneities, and minor crystalline phases, including precipitates.

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## 51c. Next Generation Radioisotope Handheld Identifier

Current scintillator-based radioisotope identifiers that use sodium iodide often do not perform well in a number of nonproliferation and safeguard applications. Although newer identifiers based on lanthanum bromide generally perform better, they are much more expensive and their performance at lower energies is actually inferior to sodium iodide. Recently, several new compounds have been identified that not only have a resolution comparable to lanthanum bromide, but also have improved proportionality and the potential for much lower cost. Thus, grant applications are sought to utilize these new materials to produce a next generation isotope identifier. In addition, it is highly desirable that proposed identifiers (1) utilize a solid-state alternative to a photomultiplier tube, and (2) contain sufficient computational power to allow a sophisticated, high confidence, isotope identification algorithm. Phase I should develop a clear system design with a quantitative assessment of the performance that would be achieved with this instrument. Phase 2 should involve the construction of a prototype instrument.

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## 51d. Next Generation Neutron Detector

New solid materials capable of detecting neutrons and distinguishing them from gamma rays are being developed, notably organic crystals grown from solution. Industrial-scale development of such technology would be a fruitful area for proposals to demonstrate instruments that exploit such materials. Important criteria for such devices are intrinsic efficiency for fission spectrum neutrons and pulse timing precision, as well as good gamma rejection ratio. Phase 1 would establish a pathway to production of significant quantities of detector material, while making use of materials supplied by NNSA laboratories. Phase 2 would expand the technology beyond the scale of individual exploratory experiments to the stage of employing kilogram quantities of high quality neutron detecting material in large detectors or arrays of modules.

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## 51e. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas relevant to this Topic.

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## 52. GLOBAL NUCLEAR SAFEGUARDS RESEARCH AND DEVELOPMENT

The Global Nuclear Safeguards Program supports NNSA's nuclear nonproliferation mission by developing innovative safeguards technologies to enhance verification of nuclear materials and activities. The program develops technologies to detect diversion of nuclear material from declared facilities; to detect undeclared nuclear material and activities; and to verify compliance with arms control treaties and agreements related to the control, production, or processing of nuclear material. The program includes R&D in nuclear (and relevant nonnuclear) measurements; information integration, and management; advanced tools for systems analysis; authentication, and containment, and surveillance.

## **52a.** Safeguards Measurement Sensors

Grant applications are sought to develop technologies to enable the dramatic improvement of safeguards measurements, both nuclear and nonnuclear. Technologies of interest include (1) an enabling technology for sensor survivability in high radiation environments, (2) an enabling technology to reduce power requirements for remote monitoring, (3) enabling manufacturing

techniques for innovative radiation sensors, (4) enabling information-processing techniques for multiplexed sensors or for the integration of large datasets. Grant applications must show a clear link between the proposed technology and the improvement in safeguards measurements.

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#### 52b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas relevant to this Topic.

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- 2. "The US Support Program to IAEA Safeguards", Modified June 5, 2008. (URL: http://www.bnl.gov/ISPO/ussp.asp).
- 3. Safeguards R&D Program in the United States presented at the 50th Anniversary meeting of Institute for Nuclear Materials Management, July 2008.

## 53. ADVANCED SIMULATION, ALGORITHMS AND MODELING

NA-22's Simulation, Algorithm and Modeling (SAM) Program supports the other programs within NA-22 by developing and exploiting models, simulations, advanced data processing concepts and algorithms to enable the detection and assessment of nuclear proliferation activities. SAM invests in high-impact, long-term, and high-risk theory, information science and technology research for facility modeling, geospatial analysis to transition between images and semantic meaning, advanced spectroscopic analysis and integrated modeling.

## 53a. Utilizing Human Computing to Annotate Geospatial Imagery

Training algorithms for image recognition require annotation of imagery, an expensive and laborious process requiring thousands of hours of time investment by the GS analysts. This project should develop a logistic framework enabling rapid parallel human annotation of geospatial imagery, design a set of tasks with challenges leading to a high quality annotation revealing the desired feature set in the imagery, create a set of imagery to test the resulting system, and conduct preliminary testing. When correctly presented using a gaming representation, the process of annotation could become easier and more engaging.

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## 53b. Advanced Graphical Data Extraction

Often the most important information in a technical document is contained in graphs of data. OCR has existed for more than 30 years and commercially available products read a wide variety

of fonts and languages. However, OCR does not accurately read important components of technical documents such as graphs and equations. Thus, applications are sought for graphical data extraction with advanced technical optical character recognition (OCR) that would add the ability to read and extract quantitative information from graphs embedded in technical documents. Graphs are usually composed of basic components, such as plotted data points, axes with numbers and text that identify the variables being plotted and curves that are fitted to the data. The desired output of this advanced algorithm would be digital arrays containing matched pairs (x, y) of data points with column headings derived from the axes of the graphs.

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## 53c. Technological Dependency Database

Applications are sought to understand how technologies depend on other technologies. NNSA seeks theory for connecting a taxonomic hierarchical list of technologies with directed edges based on direct dependency. For example, electronic micro-fabrication depends on technology for growing inexpensive high purity Si polycrystalline materials. Due to the potentially very large task of compiling the above dependency data structure, NNSA is interested in both methods for automation in the dependency edge discovery as well as specific technology taxonomies.

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#### 53d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas relevant to this Topic.

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- 1. Seneviratne, L., "Image annotation through gaming (TAG4FUN)."
- 2. Rong Yan, "An Efficient Manual Image Annotation Approach based on Tagging and Browsing."

#### 54. NUCLEAR DETONATION DETECTION

The Office of Nuclear Detonation Detection is responsible for the research and development necessary to provide the U.S. Government with capabilities for monitoring nuclear explosions. The optical waveform of atmospheric nuclear detonations is well understood and provides a way to quickly and positively identify that a detonation is nuclear. Optical waveforms from nuclear detonations are also a basis for an estimate of yield. Modern off-the-shelf electronics and networking infrastructure should make possible the production of low-cost systems for these purposes that could be widely fielded, including on buildings, towers, or vehicles.

# 54a. Time History of Optical Emissions

Grant applications are sought for ground-based systems that would detect and record the time history of optical emissions from a nuclear detonation (NuDet) in the atmosphere within 1 km of the surface. The system should consist of low-cost sensor and processing components. Consider yields of 20KT (See Glasstone, Figure 2.123 p. 69) and below, which must be measured both day and night within an environment that includes signals from natural and anthropogenic sources. The sensor system should permit economical balancing between networks with widely distributed but inexpensive sensing, reporting, and processing capability versus more elaborate and expensive point-specific capabilities. The statement of work should include proposing possible architecture, providing candidate sensor, recording, and processing nodes, acquiring background measurements, and demonstrating potential signal discrimination.

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## 54b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas relevant to this Topic.

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#### REFERENCES

1. S. Glasstone and P.J. Dolan "The Effects of Nuclear Weapons", Third Edition, United States, Department of Defense and the United States Department of Energy, (1977).

## 55. RADIONUCLIDE MONITORING FOR NUCLEAR EXPLOSIONS

The Ground-based Nuclear Explosion Monitoring Research and Development (GNEM R&D) Program in the Office of Nuclear Detonation is sponsored by the U.S. Department of Energy's National Nuclear Security Administration's Office of Nonproliferation Research and Development. This program is responsible for the research and development necessary to provide the U.S. Government with capabilities for monitoring nuclear explosions. The mission of the GNEM R&D Program is to develop, demonstrate, and deliver advanced ground-based seismic, radionuclide, hydroacoustic, and infrasound technologies and systems to operational agencies to fulfill U.S. monitoring requirements and policies for detecting, locating, and identifying nuclear explosions (see Reference 1). Within the context of one or more of these technologies, research is sought to develop algorithms, hardware, and software for improved event detection, location, and identification at thresholds and confidence levels that meet U.S. requirements in a cost-effective manner. Superior technologies will help improve the Air Force Technical Applications Center's (Reference 2) ability to monitor for nuclear explosions, which are banned by several treaties and moratoria. Annual research progress of the GNEM R&D program is available in proceedings posted on-line (see Reference 3).

Grant applications responding to this topic must (1) demonstrate how proposed approaches would complement, and be coordinated with, ongoing or completed work; and (2) address the manufacturability of any instruments or components developed.

# 55a. Improved Xenon Collection

Xenon collection systems consist of a several gas processing elements, including; preconcentration, separations, and purification stages. All of these processes require special gas handling components that are not readily available as commercial off-the-shelf items. This focus area is aimed at addressing the challenges of processing gas in each of these sub-systems where a key specification is the reduction of contamination by using gas-tight pumps. Grant applications are sought for innovative solutions to improve high-volume air sampling, gas separation and transfer in xenon collection systems. Gas transfer and separation components of interest include small, gas-tight, oil-free compressors; vacuum pumps; and gas transfer syringes:

Compressors should be capable of up to 40 liters per minute continuous flow at 5 to 7 barg (Bar, gauge pressure), gas-tight, and oil free, and should operate on 120 VAC (50 and 60 Hertz). Compressors should be designed for continuous duty, for durations in excess of 6 months prior to any compressor maintenance. Physical dimension less than 12" x 12" x 12" and less than 30 lbs.

- Similarly, small volume, gas transfer pumps should be small and gas-tight, and should achieve ultimate vacuum (<0.1 Torr) on the inlet while also compressing the output to 4 5 barg. The transfer pump should be powered by either 24 VDC or 120 VAC (50 and 60 Hertz). The desired application is to transfer gas (at atmospheric pressure) from a 1 liter sample container (down to a final pressure of 0.1 Torr) into a secondary smaller container (or equivalent) to a pressure of 4 5 barg in less than 2 minutes.
- For relatively small volume transfers (<1 standard liter of gas per cycle), transfer pumps may be in the form of a syringe-style pump or a continuous-duty mechanical design. The envisioned application would have a ~ 1 liter syringe draw sample from a container or transfer pump and then redirect it, at higher pressure, to another process stream. The external leak rate under either vacuum or pressure should be less than 0.01 standard cm³ of air / sec. Optimal factors for these components include gas-tightness, durability, operation at 120 VAC or DC power, and the ability to be contamination free (i.e., minimal use of low vapor pressure lubricants). A demonstration of the mean time between failure (MTBF) specifications is highly desirable (although due to the short time duration of the phase I portion of the project at defendable approximation to the MTBF is suitable).

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# 55b. Stable Xenon Quantification Module Development

Grant applications are sought for the quantification of the amount of stable xenon in a gas sample undergoing nuclear activity analysis, as part of a radioxenon monitoring instrument. Conceptually, a mixture of xenon in nitrogen (or helium) will be volumetrically expanded out of a small volume nuclear detector (4 cc's) into an evacuated quantification manifold. The anticipated quantity of xenon available for the measurement is 0.25 cm<sub>3</sub> (standard temperature

and pressure). The amount of nitrogen (or helium) is anticipated to be in the range of 0.25 - 0.75 cm<sup>3</sup> (STP). The objective is to derive the amount of stable xenon in this gas sample from independent measures of pressure, temperature, and mole fraction of xenon in order to calculate the stable volume (standard cubic centimeters). Therefore the quantification system should include a high quality pressure transducer, temperature probes and binary gas analyzer. Important specifications include:

- The physical volume of the system should be accurately known with low uncertainty (<1%).
- The combined relative uncertainty (random and systematic) in the reported xenon volume should be less than 3% ( $1\sigma$ ).
- The technology should be robust, field deployable and not require regular calibration (6 months between calibration checks).

This measurement is challenging due to the low pressures expected during the quantification, placing constraints on the binary gas analysis technique, therefore it is expected that new gas sensing technologies will be developed under this project.

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# 55c. Remote Field Radioxenon Monitoring System

Grant applications are sought for the development of a deployable system capable of continuous environmental monitoring for 133Xe and 135Xe via gamma detection. Each node should consist of a robust, fieldable gamma detector (e.g., CsI or NaI), acquisition electronics and data analysis algorithms. Data analysis should consist of both gross count and spectral identification. The system should have the option of transmitting data packets to a central location via wireless technology in addition to manual data transfer. An integrated data management tool should also be included allowing for rudimentary data manipulation and display. Specifications include:

- Gamma detection of 80 keV photon from 133Xe and 250 keV photon from 135Xe
- Detection of ~100 mBq/m³ levels are desired but detection of 5 Bq/m³ or lower are acceptable
- Portable detector for short term installation
- GPS enabled for time and location input
- Low Power

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## 55d. Medical Isotope Stack Monitoring

Understanding the gaseous radionuclide emissions from Medical Isotope production facilities is an important element in quantifying sources of background relevant to nuclear explosion monitoring.

Grant applications are sought for an integrated medical isotope stack monitoring system. The system should be capable of determining the activity of a range of radionuclides via spectroscopy using automated peak fitting routines. In addition, stack flow rates shall be used to compute the activity concentration of the radionuclides (i.e., Bq/m3 effluent). A secondary dilution system

may be used to reduce the high activities expected during production intervals, this additional dilution must also be factored into the calculation of activity concentration. Software database management tools should be included allowing for efficient data archiving and analysis. Specific requirements are listed below:

- Important Radionuclides: <sup>131m</sup>Xe, <sup>133</sup>Xe, <sup>133m</sup>Xe, <sup>135</sup>Xe, <sup>85m</sup>Kr, <sup>131</sup>I, <sup>133</sup>I and <sup>135</sup>I
- Stack flow rate input
- Flow rate and dilution monitoring through detector
- Automated peak fitting, radionuclide identification and variable integration time
- An additional filtering system (e.g., charcoal or particulate) for iodine with its own separate detector system will likely be necessary.
- System must have high dynamic range, from background (10<sup>3</sup> Bq/m<sup>3</sup>) to high release levels ~10<sup>12</sup> Bq/m<sup>3</sup> (added range up to 10<sup>14</sup> Bq/m<sup>3</sup> would be desirable)

Measurement precision of +/- 10%

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# 55e. Cryogenic Thermal Break

Mechanical cryogenic coolers can greatly improve the efficiency of a xenon collection system. Coolers can be used in all of the important sub-systems, including pre-concentration, separations and purification. The amount of cooling (i.e., thermal lift) and temperature varies for each of these separate processing steps. For many gas processing schemes it is common to operate the component attached to the cooler at low temperature for adsorption and then heat the same component to high temperature to desorb the previously adsorbed species. One technical challenge that can limit design options is the *maximum allowable* temperature of the coolers cold-head when not in operation; many of these cold-heads are rated to 50 C or less. For maximum flexibility it is desirable to heat gas adsorption components to temperatures in excess of 250 C.

Grant applications are sought for a cryogenic thermal break, defined as a device mounted to a mechanical cooler's cold-head that allows maximum thermal lift during the cold cycle and minimizes thermal conductance to the cold-head during heating. The device should:

- Adaptable to fit a variety of cold-heads whose diameter ranges from 1" to 3".
- The working end of the device should allow for a variety of mounting options for attaching different components (e.g., a series of mounting holes on a flat platform).
- Should operate from -200 C for cooling applications and up to +300 C for heating applications.
- Device itself should be as compact as practical and have minimal ancillary control equipment.
- Able to operate at atmospheric pressure in an insulated enclosure.
- Will be attached to coolers with thermal lift in the range of 2-3 Watts at -200C up to a 100 Watts at -50C.
- The time scale between thermal short and thermal open should be less than 5 minutes.
- The device should be able to operate without maintenance for at least 1 year with thermal cycling 4 times per day.

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#### 55f. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas relevant to this Topic.

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#### REFERENCES

1. "Nuclear Explosion Monitoring Research and Engineering Program Strategic Plan, National Nuclear Security Administration," September 2004. (Document No. DOE/NNSA/NA-22-NEMRE-2004) (Full text available at

https://na22.nnsa.doe.gov/cgi-bin/prod/nemre/index.cgi?Page=Strategic+Plan)

- 2. U.S. National Data Center, Air Force Technical Applications Center, http://www.tt.aftac.gov/wrt/
- 3. Annual Research Review Proceedings for Ground-Based Nuclear Explosion Monitoring Research and Engineering, sponsored by the National Nuclear Security Administration and the Air Force Research Laboratory. (Available at: https://na22.nnsa.doe.gov/proceedings)

## **56. COMPACT SEISMO-ACOUSTIC MONITORING SYSTEM**

Growing efforts to study explosion monitoring in the local range (0 to 200 km) have identified a need for an improved and simplified sensor package. What would be useful is a compact system to record 3 components of seismic motion as well as acoustic pressure.

# 56a. Meet Current Industry Standards for Seismic Recording

Grant applications are sought for seismo-acoustic recorders that meet current industry standards for seismic recording. The recorder characteristics should meet current industry standards for seismic recording: 24 bit resolution, high dynamic range (> 120 dB), precise timing (accuracy better than 0.001 s), high sample rate (up to 2 kHz) and environmentally stable (at least -20 to +50 C, watertight, etc.).

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## 56b. High Fidelity Sensors with Telemetry Connectivity

Grant applications are sought for high fidelity seismo-acoustic sensors with telemetry connectivity. The sensors should be high fidelity, have a broad frequency response appropriate for recording explosions in the local range (approximately 0.1 to 1000 Hz), and handle a dynamic range from low noise background to the higher amplitudes expected in the near field (perhaps as high as 0.1g acceleration equivalent for seismic motion). It should be possible to connect the recorder to telemetry.

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## 56c. Small, Light Package with Low Power Consumption

Grant applications are sought for a small, light recording system with low power consumption. The entire package should be small and light (a single installer/individual should be able to carry a few complete systems) but be capable of recording continuously for up to a year. Low power consumption is very important.

Contact: Leslie Casey, 202-586-2151, leslie.casey@nnsa.doe.gov

## 56d. Continuous and/or Triggered Recording

Grant applications are sought for continuous and/or triggered seismic recording. The recorder should operate in continuous recording and/or triggered modes, and the user should be able to select the mode to be sent to a telemetry system. Innovative sensors that would support such a package are also of interest.

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## 56e. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas relevant to this Topic.

Contact: Leslie Casey, 202-586-2151, leslie.casey@nnsa.doe.gov

#### REFERENCES

1. L.A. Casey and W.R. Bell, "Nuclear Explosion Monitoring Research and Development Roadmaps," Proceedings of the 2010 Monitoring Research Review, September 2010 (Available at: https://na22.nnsa.doe.gov/mrr/2010/PAPERS/01-01.PDF).

## 57. ADVANCED SEPARATIONS CHEMISTRY TOOLS

Separations chemistry is practiced broadly for a variety of applications related to DOE missions. These applications range from environmental sampling and analysis of trace constituents for nuclear forensic analysis of radioactive samples. New chemical separations methods are needed to enable researchers to rapidly and reproducibly isolate several chemical species of interest that are in liquid mixtures at relatively low concentrations. Advances in technical tools that perform efficient separations can directly impact the pace and extent of scientific study of species that are in low concentrations but whose presence, if detected and quantified, has significant diagnostic value.

# 57a. Development of Resin Material Binders Compatible with Emerging Highly Selective Ligands

Extractions that now use the ligand 4-chloro-2-[(6-chloro-7-methyl-2H-1,3-benzoxazin-3(4H)-yl)methyl]-5-methylphenol, and related ligands, are of interest to perform in ways that are more efficient – that is, that are more rapid, and that achieve a high degree of separation between the analytes that this ligand sequesters and other species in the original liquid mixture. These efficiencies can be obtained by the development and use of an appropriate resin (binder) material that is compatible with this ligand and that enables it to be used in a column, for use in extraction chromatography.

Currently this ligand is used in a solvent extraction (SX) method. SX is not a rapid method of separation, nor is it an environmentally friendly process as large amounts of toxic solvents are used. The binding of this ligand to a solid support would greatly increase the ease and speed of the separation.

Grant applications are sought for the development of a resin material that incorporates this ligand in the surface area of an extraction column. Properties of interest include minimal degradation of the ligand performance in its degree of separations (e.g., as measured by decontamination factors in comparison to SX or batch mode tests), flow-through rates, and the rapidity of separations achieved with the new resin. The references below describe the synthesis of this ligand type and initial data on the SX of the ligand for Ga(III).

Contact: Tom Kiess, 202-586-7664, Thomas.kiess@nnsa.doe.gov

# 57b. Automated Evaporation of Aqueous Acidic Solutions

Aqueous-based separations are used widely, in applications that include medical isotope production and the isolation of trace species of interest in nuclear forensics analyses. These methods rely on the transposition of solutions between separation steps. An automated system that can rapidly transpose many solutions without cross-contamination would improve the timeliness and fine-tuned control that can be applied to many separations processes. A major time- and labor-intensive step in aqueous-based separations of various elements often is not the separation itself, but rather the conversion of the carrier solvent from one type to another. This conversion typically involves evaporating an aqueous solution to dryness and reconstituting the remaining solute residue in another solvent matrix. This evaporation is done under controlled conditions because of the need to carefully ensure the solvent is fully evaporated while the solute product of interest is not destroyed by overheating. This controlled evaporation is a process that could be automated.

Grant applications are sought for the development of an instrument designed to drive off water and acid from a sample (through heating or another method) under automated control. Such a system would need to be compatible with various acid vapors (specifically to include HNO3, HCl, HF, and HClO4). Important features are the sample throughput and routing of off-gases – so as to be able to process large numbers of samples (e.g., as many as 24, each of volume 0.1-10 milliliters) without cross contamination between them.

Contact: Tom Kiess, 202-586-7664, Thomas.kiess@nnsa.doe.gov

## 57c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas relevant to this Topic.

Contact: Tom Kiess, 202-586-7664, Thomas.kiess@nnsa.doe.gov

## **REFERENCES**

## Subtopic a:

- 1. Hirayama, N. Horita, Y. Oshima, S. Kubono, K. Kokusen, H Honjo, T. Selective Extraction of Gallium (III) Using Tris(2-hydroxy-3.5-dimethylbenzyl)amine, *Analytical Sciences* 2001 *17*, 257-260 and references therein.
- 2. Hultzsch, K. Chem Ber, 1949 82, 16 ff.
- 3. Komissarova, N. Belostotskaya, I. Shubina, O. Ershov, V. Vosnesenski, V Chervin, I. Anamalous Duff Reaction with 2,4-di-tert-butylphenol. *Institute of Physical Chemistry, Academy of Sciences of the USSR, Moscow (Engl. Trasl.)* 1988; *Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya*, 1988 9 2186 ff.

# **Subtopic b:**

- 1. United States Patent 4604363
- 2. United States Patent 5514336